

MUSE: Multi-algorithm collaborative crystal structure prediction

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(Dated: March 14, 2013)

The multi-algorithm collaborative crystal structure prediction was realized and constructed as a Multi-algorithm-collaborative Universal Structure-prediction Environment (MUSE). The evolutionary algorithm was coupled with the simulated annealing and the basin hopping algorithms to efficiently find the stable and metastable structures of materials under certain conditions. After introduced two new operators, slip and twist, the diversity of structures are exceedingly enhanced. In particular, in order to achieve the self-adaptive evolution of structures, MUSE uses the competition techniques of ten variation operators to increase the diversity of crystal structures. The multi-algorithm coupling, the ten variation operators, the symmetry constraints in the first generation and the self-adaptive algorithms are all key techniques to improve the search efficiency of MUSE. To show the search ability of MUSE and how it works, I presented some predicted systems including metallic, covalent and ionic systems. All the test results show MUSE has high efficiency and almost 100% success rate.

I. INTRODUCTION

The structure of a material provides key information for us to conveniently and deeply explore its properties. Especially, the first-hand structure information is the beginning to discover new physics and chemistry of materials in extreme environments. Commonly, the structure information can be achieved from experiment via the X-ray powder diffraction technique. However, when the material is in very complex or extreme conditions such as high pressure and/or high temperature¹ or its composition is beyond our chemical intuition,² experiment is often difficult or even impossible to identify its structure. On the contrary, the theoretical method is often efficient, economic and convenient. Even though Madox claimed the “scandal in the physical sciences” of the inability to predict the structures of materials from stoichiometry two decades ago,³ up to date many groups have made great success in structure prediction only from stoichiometry based on different stochastic search algorithms, including the simulated annealing,⁴ the minima hopping,^{5,6} the basin hopping,⁷ the evolutionary algorithm,^{1,2,8,9} the particle swarm optimization,^{10,11} and the random search.¹² Utilizing these methods, many groups have found plenty of novel materials under ambient and extreme conditions.

The evolutionary algorithm was inspired by biological evolution, such as mutation, reproduction, recombination, and selection. The whole population’s evolution is the process of the survival of the fittest. For the crystal structure prediction, this algorithm is utilized by introducing several evolutionary operators. The evolution speed is determined by the evolutionary operators including the variation operators and the selection operator. The variation operators control the diversity of the population, and the selection operator mainly determine the direction of evolution. The simulated annealing algo-

rithm was from annealing in metallurgy, which hastens a melted material to be crystal by controlled cooling. Simulated annealing improves its efficient through the introduction of two tricks: the so-called Metropolis selection rule¹³ and lowering the “temperature”. The basin hopping algorithm is just as its name that means trying to escape the local minima by hopping. The basin hopping algorithm also uses Metropolis rule.¹³

The optimization algorithms are all stochastic techniques and have their own inherent advantages and disadvantages. If we can organically combine some of these algorithms to let them work collaboratively, we will avoid the disadvantages and fully utilize their advantages. In MUSE, I organically combined the evolutionary, the simulated annealing and the basin hopping algorithms to collaboratively predict the stable and metastable structures of materials.

The implementation of multi algorithms collaboration are based on the manipulation of crystal structures in real space, i.e. the operations on crystal structures made by the variation operators. So in order to manipulate crystal structures conveniently, the structure of crystal is described by the shape of the lattice cell and the atoms positions therein. The fitness for the survival of the best is the free energy of each structure. The structure with lowest free energy have the best fitness. Thus, the selection operators is to select lower free energy structures (parents) to generate new structures (offspring). We also refer to each structure as an individual and all the structures as the population.

In this paper, I focus on the implementation of the multi algorithms collaboration technique and how it works. This paper is organized as follows. Section II is the algorithms implementation. This includes multi algorithms collaboration, the descriptions of the evolutionary and variation operators, the evaluation and selection of an individual and how the search is terminated. I will show some results predicted by MUSE in Section III. The

predicted systems includes metallic, covalent and ionic systems. The discussion and conclusion are provided in Section IV.

II. ALGORITHM IMPLEMENTATION

MUSE is developed for easy use in structure prediction of materials under ambient or extreme conditions, e.g. high pressure. It was written in Python and organically combined the multi algorithms including the evolutionary algorithm, the simulated annealing algorithm and the basin hopping algorithm to collaboratively search the global energy minima of materials with the fixed stoichiometry. After introduced the competition in all the evolutionary and variation operators, the evolution of the crystal population and the choice of the operators are self-adaptive automatically. That is to say the crystal population undergoes a self-adaptive evolution process. So, it can effectively find a material's stable and metastable structures under certain conditions only provided the chemical information of the material.

MUSE depends on external local optimization codes. At present, MUSE uses VASP,^{14,15} SIESTA,¹⁶ Quantum ESPRESSO¹⁷ and LAMMPS¹⁸ as the local optimization tools. It determines the space group number of each optimized structure immediately after the optimization is done. The duplicate structures are then eliminated according to the space group numbers and the enthalpies. In detail, the supercells with the same space group number are first reduced to primitive cells. Then the duplicated structures are deleted if the numbers of atoms in the primitive are equal and their enthalpy difference are less than 1 meV/atom. More importantly, MUSE generates the random structures of the first generation with symmetry constraints, which largely shortens the optimization time of the first generation and increase the diversity of crystal population. The random structures are created according to the randomly chosen space group numbers from 2 to 230 and Wyckoff positions must be fit to the atom numbers ratio of different kinds. Especially for large systems, the constraints on symmetry will avoid the unphysical disorder crystal structures, similar to glass state. MUSE can also pick up (restart) a previous interrupted search from wherever the search stopped.

A. Multi-algorithm collaboration

A single algorithm has more or less inherent disadvantages. Using the combination of multi algorithms, or hybrid, we will avoid their disadvantages and effectively make use of their advantages. The efficiency of the multi-algorithm collaboration search also depends largely on the diversity of crystal population, which is up to the evolutionary and variation operators. To increase the

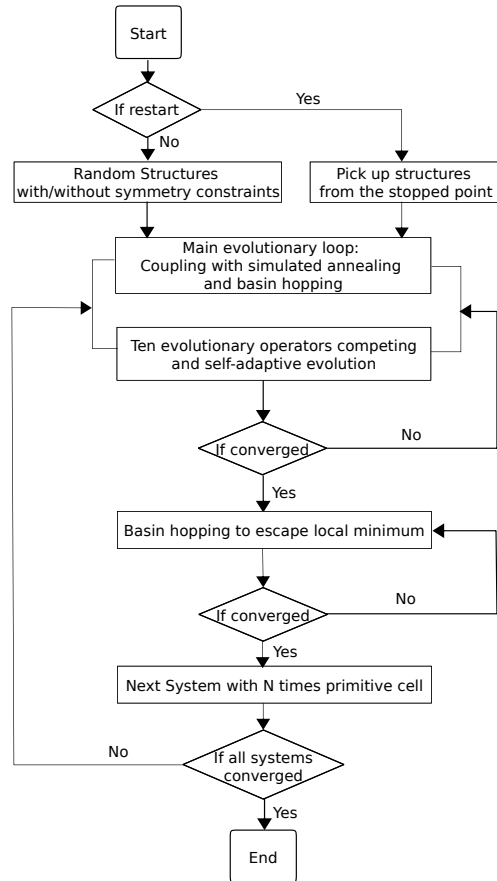


FIG. 1: The flowchart of multi algorithms collaboration and coupling in MUSE

diversity of crystal structures, MUSE uses ten evolutionary and variation operators, including cross over, mutation, permutation, cross-over-mutation, permutation-mutation, slip, twist, random move, ripple and mutation-ripple. The multi-algorithm collaboration and coupling are shown in Fig. 1. Different systems have different optimal operators to achieve the possible largest diversity. So, from the second generation these ten evolutionary operators will compete with each other in their success rates starting from the initial value 100% of each operator. The operators are randomly used according to their historical behaviors from the third generation. That is to say, the more positive contributions (produced lower enthalpy structures or increased the diversity) an operator has done to the whole population previously, the more chances it will have to be called to breed offspring. This is called the self-adaptation of evolutionary operators for different systems, which turns out to largely increase the diversity of structures and hasten the convergence of global search.

Whether the new optimized offspring in the main

evolutionary loop is kept or not is determined by the Metropolis algorithm¹³ based on the decreasing temperature, which actually couples the evolutionary algorithm and the simulated annealing algorithm together. Furthermore, to prevent prematuration, the main evolutionary loop is also coupled with basin hopping algorithm which has advantage of global optimization. After the main evolutionary loop is converged, MUSE will enter into the pure basin hopping loop to try to escape the possible local minimum. Tests show if we gather the structure information from the small systems with small number of primitive cells, we will easily convergence the large systems who have more primitive cells. So we are encouraged to start from small systems with small number of primitive cells. This process is automated in MUSE. If all the systems are converged, MUSE will terminate the search and exit.

B. The first generation

A unit cell in MUSE is described with six parameters, \mathbf{a} , \mathbf{b} , \mathbf{c} , α , β and γ , and the atoms positions, where \mathbf{a} , \mathbf{b} and \mathbf{c} are the lattice vectors and α , β and γ are the corresponding angles as normal. The structures of the first generation can be randomly created with the symmetry constraints by randomly choosing crystal space group number (with Wyckoff positions constraints) from 2 to 230 and the constraints of the minimum and maximum angles (45° and 135°) between lattice vectors. Or, if one wants to generate the first generation in the fully random manner, MUSE will generate the structures without symmetry constraints but still with the constraints on minimum and maximum angles between lattice vectors. Then its volume is scaled to the coarsely guessed one with the constraints of the minimum length of lattice vectors and the minimum distance between atoms. If a space group number is used once, MUSE will try to avoid using it for the rest of the random structures in order to prevent duplication and increase the diversity.

C. Evolutionary and variation operators

The individuals in the second generation are created using the evolutionary and variation operators from the certain percentage of the number of individuals in the first generation. The ten operators fall into two categories: the single-parent based operators and the two-parent based operators. The mutation, the permutation, the random move, the ripple, the slip, the twist, the permutation-mutation and the mutation-ripple operators are all the single-parent based operators. The cross over and the cross-over-mutation operators are two-parent based operators.

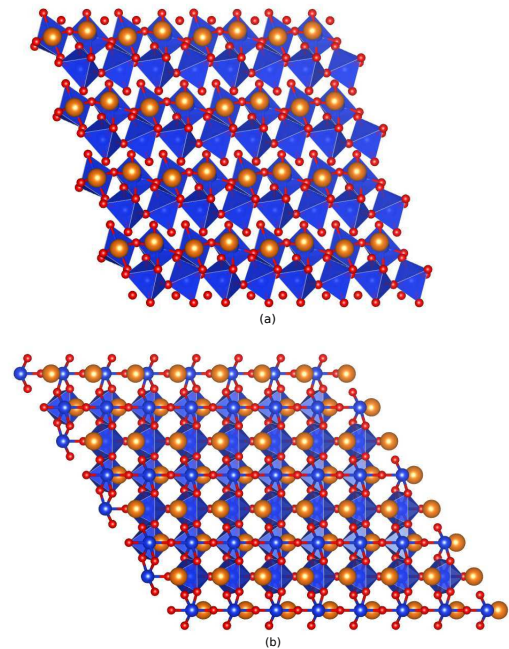


FIG. 2: The example of mutation. (a) Randomly chosen parent: P-1 (2), (b) Offspring: P2₁/m (11). The two structures are locally optimized.

1. Mutation

The mutation operator variate one selected parent to produce a new individual (offspring) by multiplying the unit cell row vector with a symmetric Voigt strain matrix:^{1,2,19}

$$\mathbf{a}' = \begin{bmatrix} 1 + \delta_{11} & \delta_{12}/2 & \delta_{13}/2 \\ \delta_{12}/2 & 1 + \delta_{22} & \delta_{23}/2 \\ \delta_{13}/2 & \delta_{23}/2 & 1 + \delta_{33} \end{bmatrix} \mathbf{a}, \quad (1)$$

where δ_{ij} are the zero-centered Gaussian random variables with a specified standard deviation. \mathbf{a} is the original lattice vector, and \mathbf{a}' is the new lattice vector. The atomic coordinates are fractional values and are scaled to the new vectors. The mutation operator is actually applying a shear strain on the cell to cause it to undergo phase transition. So the mutation operator is the very effective operation to diversify the crystal population. However, different systems have different optimal standard deviations δ_{ij} , so MUSE uses trial and error scheme to obtain good diversity from the initial standard deviation value. After applying the strains the crystal's volume is then scaled to the volume of the lowest enthalpy structure in the previous generation. For the example of mutation, please see Fig. 2.

2. Permutation

The permutation operator changes the positions of two kinds of atoms a random number of times.^{1,2,19} This ob-

viously increases the diversity of the crystal population after operation. The permutation operator can only be called when the atom types is more than one.

3. Permutation-mutation

The permutation-mutation operator is the hybrid of the permutation and mutation operators. The unit cell is mutated after exchanging two atoms of two different kinds random number of times. It is the single-parent operator, but it obviously increases the diversity of the crystal population.

4. Random move

The random move operator only randomly moves the atoms positions by random amount, keeping the lattice vectors unchanged. It displaces the three fractional coordinates of all atoms by random amount between $[-D_{\max}, D_{\max}]$, where D_{\max} is the maximum percentage of coordinates that atoms displaced. The use of this operator combined with the Metropolis algorithm realized the basin hopping loop.^{7,13} The periodic boundary conditions are applied after randomly moved atoms. This loop is coupled with the main evolutionary loop.

5. Slip

To fully variate the crystal structure, MUSE introduced a new operator slip. The slip operator let a group of atoms slip by a random distance along a random direction that is parallel to a specific plane. This operator comes from the real crystal phase transition process in which some atom layers or atoms slip along special direction. So it will considerably increase the diversity of crystal structure.

6. Twist

The twist operator is also a new operator first constructed in MUSE. It twists the supercell by rotating atoms along the randomly chosen axis. After this operation atoms will be rotated by $\theta_0 + \Delta\theta$ around the chosen axis, where $\Delta\theta$ is the interval of rotated angles between different atoms. Twist often causes phase transition in real crystal under extreme conditions. So it also a high efficiency operator.

7. Ripple

The ripple operator, first proposed by Lonie and Zurek,² is the periodic displacement operator which shifts

the coordinates of each atom along a randomly chosen axis by certain amount. For example, if x -axis is chosen, the x components of all atoms will be shifted to the new values in fraction: $x_{\text{new}} = x + \Delta x$, where Δx depends on the atoms non-displaced (i.e. y and z) coordinates via:²

$$\Delta x = \rho \cos(2\pi\mu y + \theta_y) \cos(2\pi\eta z + \theta_z), \quad (2)$$

where ρ is the maximum possible displacement in x direction, and μ and η are integers, and θ_y and θ_z are random numbers between $[0, 2\pi)$.

The ripple operator is also a single-parent operator, but it can substantially increase the crystal diversity. Some solids manifest the ripple motif at ambient or high pressure, such as Cs-III,²⁰ Rb-III²¹ and Ga-II.²² Fig. 3 is an example of ripple.

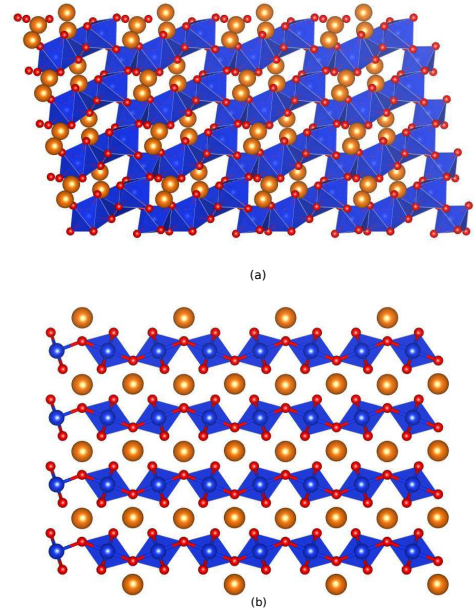


FIG. 3: The example of ripple. (a) Randomly chosen parent: P1 (1), (b) Offspring: Cmcm (63). The two structures are locally optimized.

8. Mutation-ripple

This operator is the hybrid of the mutation operator and the ripple operator. The unit cell is acted by the ripple operator after it is mutated.

9. Cross over

The cross over operator is the two-parent based operator. It cuts and splices the randomly picked two parents to make a new offspring.^{1,2,19,23-28} It mainly consists of

two steps: cut and splice. In the first step, the cut plane is parallel to the randomly not picked two vectors of one randomly picked parent and the cut position is in the 0.5-centered Gaussian random number between $[0.25, 0.75]$. If the atoms coordinates of the picked axis is below the Gaussian random number, they are taken as the part of the new individual. The other part of the new individual is from the other parent in the same way but the atoms coordinates are larger than the same Gaussian random number. In the second step, the picked atoms from the two parents are placed together to make the atoms coordinates of new individuals. The new lattice vectors are the vectors summation of the two parents. To increase the success rate and effectiveness, the atoms are centered before cross over operation. Fig. 4 is one example of cross over.

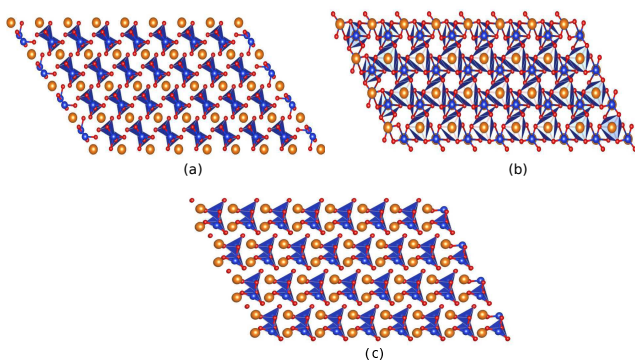


FIG. 4: The example of cross over. (a) Randomly chosen parent 1: Cmmm (63), (b) Randomly chosen parent 2: P6₃/m (176), (c) Offspring: Pm (6). The three structures are all locally optimized.

10. Cross-over-mutation

The cross-over-mutation operator is the hybrid of the cross over operator and the mutation operator.

D. Evaluation and selection

As other stochastic structure search algorithms,^{1,2,8,10-12} MUSE also uses *ab initio* Gibbs free energy as the fitness function, which evaluates if an individual is suited to be parent to breed offspring. At 0 K, Gibbs free energy equals to enthalpy. The enthalpy ($H = E + PV$) of an individual is determined from the local optimization code. The absolute probability p_i of an individual being selected for breeding offspring is

determined by

$$p_i = \frac{H_{\max} - H_i}{H_{\max} - H_{\min}}, \quad (3)$$

where H_i is the enthalpy of this individual, and H_{\max} and H_{\min} are the enthalpies of the worst and the best individuals in the last generation, respectively.

After an offspring is generated and locally optimized, whether it is kept or not is up to the Metropolis rule¹³:

- An individual is kept if its enthalpy is lower than that/those of its parent(s).
- But if its enthalpy is greater than that/those of its parent(s), it is kept only if

$$\exp[(H_{\text{parents}} - H_{\text{individual}})/kT]$$

is greater than a randomly picked number from $[0, 1]$. k is Boltzmann constant. The initial temperature T_0 for annealing is specified in the input file. The temperature in generation n is reduced to $T_n = 0.9T_{n-1}$.

E. Termination

The termination of the main evolutionary loop coupled with the simulated annealing and the basin hopping in MUSE is controlled by the terminator operator. The main loop is terminated:

- if the number of continuous generations with the best enthalpy difference less than 1 meV/atom and the same symmetry structures reaches the number specified in the input file;
- if the specified maximum number of generations has been done;
- if the diversity of the crystal population is too low.

While, the pure basin hopping loop is terminated when the loop number reaches the number of continuous generations with the best enthalpy and the same space group number.

F. K-point adaptation

The K-point adaptation is similar to Ref. 1. The K-grid in reciprocal space of a lattice vector i is calculated via:

$$k_i = \frac{1}{a_i \cdot k_{\text{resol}}}, \quad (4)$$

where a_i is the length of the lattice vector i , and k_{resol} is the reciprocal-space resolution set in the input file. k_i is then rounded to an integer.

III. RESULTS

The multi-algorithm collaboration in MUSE have been sufficiently tested for many cases including metallic, covalent and ionic systems. Table I shows the searched

TABLE I: The stable structures of different systems predicted by MUSE under different conditions. N_{atom} is the number of atoms in the system. P is the target pressure in GPa. Size is the population size in each generation. N_G shows how many generations MUSE used to find the stable structure.

System	N_{atom}	P (GPa)	Population size	Symmetry	N_G
Pd	10	0	20	$Fm\bar{3}m$	1
Ta	10	0	20	$Im\bar{3}m$	1
Au	8	0	20	$Fm\bar{3}m$	1
Nb	8	100	20	$Im\bar{3}m$	1
Y	8	140	30	$Fddd$	2
Sr	20	100	30	$C2/m$	3
C	12	50	30	$Fd\bar{3}m$	4
SiC	20	20	30	$F\bar{4}3m$	2
LiBC	12	0	30	$P6_3/mmc$	6
NaCl	20	0	30	$Fm\bar{3}m$	1
GaN	20	0	30	$P6_3mc$	2
NbN	8	100	30	$P6_3/mmc$	1
NbS ₂	18	50	30	$I4/mmm$	3
MgSiO ₃	20	130	30	$Cmcm$	5

stable structures of different systems under different conditions. The random structures in the first generation were constructed with symmetry constraints. The *ab initio* optimizations and the free energy calculations for every structure generated by MUSE were performed with VASP.^{14,15} The GGA parametrized by PBE²⁹ was applied and the electron-ion interactions was described by the PAW scheme.^{30,31} To achieve good convergences the kinetic energy cutoff and the k -point grids spacing were chosen to be 1.3 times the default values and 0.03 \AA^{-1} , respectively. As one can see, the systems with not more than two kinds of atoms are very easy for MUSE to find the stable structures; it generally finds them in not more than three generations. However, the systems with more than two kinds of atoms need at least five generations. On the other hand, in accord with our intuition larger systems take more generations to successfully find the global lowest enthalpy structures, because the configuration space increases exponentially with the system size. All the searched stable structures are in agreement with the known structures.

A. Metallic systems

Tests on metallic systems have been done for Pd, Ta, Au, Y, Nb and Sr. Except for Y and Sr, the known stable structures of other metals were found in the first generation. Y is a metal at ambient conditions. Under compression, it will exhibit superconducting properties according to recent report.³² At 140 GPa, MUSE also found the superconducting $Fddd$ phase (see Table I for details) recently reported by Chen et. al.³² Apart from the $Fddd$ phase, MUSE also found other energetically competitive structures, such as the structures with

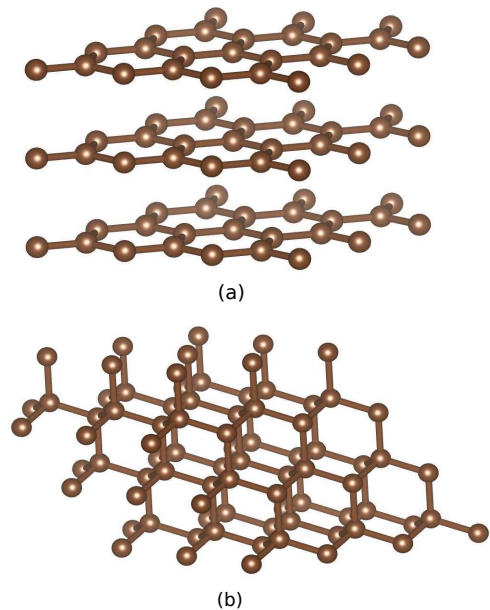


FIG. 5: The predicted structures for 12 C atoms at 50 GPa. (a) graphite, (b) diamond.

$C2/c$ (No. 15) and $P2_1/c$ (No. 14) which have not been reported before.

B. Covalent systems

The covalent systems including C, SiC and LiBC were also fully tested. After performed search for 12 C atoms at 50 GPa, MUSE successfully reproduced the diamond-C and graphite-C in the same search (see Fig. 5). The diamond phase is the most stable one. Other metastable structures with symmetries $Cmmm$ (No. 65), $Fmmm$ (No. 69), $R\bar{3}m$ (No. 166), $C2/m$ (No. 12), $P\bar{6}2m$ (No. 189) and so on, are also found. SiC with two atom types only takes three generations for MUSE to find the stable structure with space group $Fm\bar{3}m$. Many energetically competitive structures are also found, including structures with $P6_3mc$, $Ccm2_1$, $C2/m$, Cm and $P3m1$ symmetries. The enthalpy of the structure with $P6_3mc$ (No. 186) symmetry is only 3.1 meV/atom higher than that of $Fm\bar{3}m$ at 10 GPa. LiBC is an intermetallic compound which also shows strong in-plane covalent bonding. MUSE only used 6 generations to find the known $P6_3/mmc$ structure for the 12 atoms system.

C. Ionic systems

NaCl is a typical well-known ionic system. With the help of symmetry constraints on the first generation, MUSE found its stable $Fm\bar{3}m$ in the first generation using

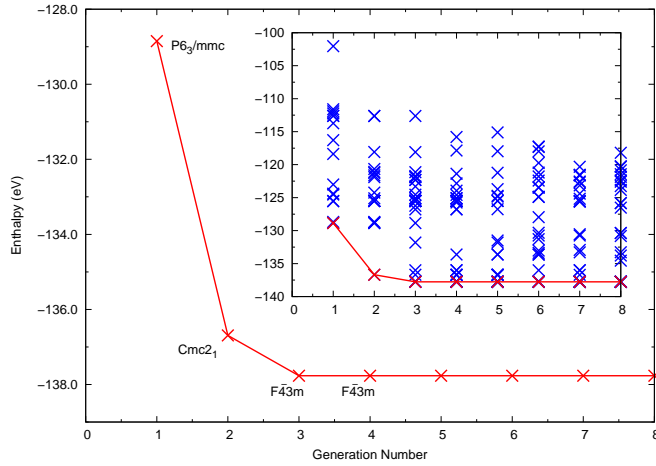


FIG. 6: The self-adaptive evolution of SiC structures at 10 GPa. The cell contains 10 atoms. The structure with $F\bar{4}3m$ symmetry was found in the third generation. The inset shows all the structures searched.

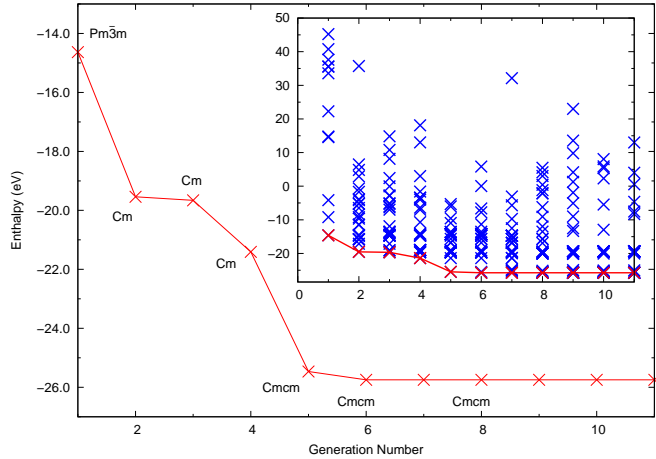


FIG. 7: The self-adaptive evolution of MgSiO₃ structures at 130 GPa. The cell contains 20 atoms. The well-known post-perovskite structure (Cmc) of MgSiO₃ was found in the fifth generation. The inset shows all the structures searched.

20 atoms. Fig. 7 shows the evolution of MgSiO₃ structures at 130 GPa. There are 20 atoms in the unit cell.

With so many atoms in the cell, MUSE find the well-known post-perovskite structure only in five generations. At the same time, MUSE produced many metastable stable structures with relatively lower enthalpies. Smaller MgSiO₃ systems with 10 atoms were also tested at 130 GPa, and MUSE only used two generations to find Cmc structure.

IV. DISCUSSION AND CONCLUSION

The implementation of the multi-algorithm collaboration for crystal structure prediction are detailed. After introduced two new variation operators, slip and twist, the search ability of MUSE are enhanced. In order to further increase the search efficiency of MUSE, the number of variation operators are also increased to ten. Furthermore, after adopting the competition scheme in the ten variation operators, different systems will find different optimal variation operators in evolution and then fasten the convergence speed. These techniques are all key to improve the efficiency of crystal structure prediction. Tests on different systems show the very high efficiency of multi-algorithm collaboration.

Using 12 C atoms, MUSE successfully reproduced the known diamond and graphite structures, apart from some energetically competitive metastable structures. As for the complex MgSiO₃ systems with 20 atoms, MUSE only used five generations to find its well-known post-perovskite phase at 130 GPa. For the metal systems, tests on Ta, Pd, Au, Y, Nb, Sr, etc, also show very high efficiency. For metal Y, MUSE found the $Fddd$ phase at 100 GPa, which was recently reported. In all tests, MUSE achieved the success rate of almost 100%. So, the multi-algorithm collaborative crystal structure prediction has high search efficiency and success rate.

V. ACKNOWLEDGEMENTS

The research was supported by the National Natural Science Foundation of China (No. 11104127), the Henan Research Program of Basic and Frontier Technology (No. 102300410213), and the Science Research Scheme of Henan Education Department (No. 2011A140019).

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